UV/Visible/Near-Infrared Reflectance Models for the Rapid and Non-Destructive Prediction and Classification of Cotton Color and Physical Indices

Y. Liu, G. Gamble, D. Thibodeaux

Abstract. *HVI, utilized in the cotton industry to determine the qualities and classifications of cotton fibers, is time consuming and sometimes destructive. UV/visible/NIR spectroscopy, a rapid and easy sampling technique, was investigated as a potential method for the prediction of such key cotton color and physical attributes as reflectance (Rd), yellowness (+b), micronaire, strength, mean length, upper-half mean length, short fiber index, and uniformity index. Cotton fibers were scanned in the region of 220-2200 nm, and HVI values were measured as the references. PLS regression models were individually developed and then compared for each property in three spectral ranges. The best performances for nearly all properties were obtained from the region covering the UV/visible absorptions, which was in consistent agreement with Pearson correlations from HVI data alone. On the basis of RPD value in the validation set, the suitability of UV/visible/NIR predictive models could be in the descending order of micronaire, +b, Rd, mean length, upper-half mean length, uniformity index, short fiber index, and strength. In addition, to limit the possibility of misclassification for boundary samples from the micronaire PLS model, a 3-class SIMCA/PCA model was developed and the classification efficiency was compared. The comparison indicated that the discrimination model utilizing the UV/visible region could assign one cotton fiber to an appropriate micronaire class of "Discount Range," "Base Range," or "Premium Range" with a success rate of 100% for the samples under investigation. Both prediction and classification results suggested that the UV/visible/NIR technique is an accurate means of determining fiber micronaire for cotton quality grading and classification.*

Keywords. *Color and physical properties, Cotton fiber, HVI, Near-infrared spectroscopy, Prediction and classification, UV/visible spectroscopy.*

Cotton is one of the most important agricultural commodities in the world, and the subsequent need for rapid and accurate determination of cotton fiber qualities is an important topic from policy makers to cotton fiber processors. Over the years, the USDA and other organizations have established cotton fiber grade and classification standards. Various techniques, including optical, physical, and chemical methods, have been developed to classify cotton fibers. Before 1960, the classification was carried out mainly by subjective hand and eye perceptions and by using objective microscopes and scales. Between 1960 and 1970, a technique known as high-volume instrumentation (HVI) measurement was introduced by the USDA to measure color and physical properties of cotton fibers such as reflectance, strength, length, micronaire, and uniformity (Gordon, 2007). At present, the HVI method, together with other recently developed instrumental methods, e.g., advanced fiber information system (AFIS) (Bragg and Shofner, 1993), has continued to be a viable tool for determining a number of effective cotton quality parameters. Although these devices can measure many different quality indices and are used throughout the cotton industry, the procedures are usually destructive, time consuming, and prone to day-to-day and location-to-location variations. Considerable efforts have been made to address several concerns about these instrumental methods, for example, the repeatability within one HVI and the reproducibility between different HVI evaluations (Knowlton, 2002a, 2002b), the relationship between HVI color parameter and globally recognized CIELAB color system (Rodgers et al., 2008), and the correlation of short fiber content from the readings of three different instruments (HVI, AFIS, and Suter-Webb array) (Thibodeaux et al., 2008).

Since HVI and AFIS methods measure the color and physical property information of cotton fibers, it will be of interest to obtain independent and complementary information on cotton fibers from other non-destructive approaches. These approaches include laser light scattering (Thomasson et al., 2009), infrared (Griffiths and De Haseth, 1986), near-infrared (Burns and Ciurczak, 2001), and Raman spectroscopy (Park, 1983). Among them, near-infrared (NIR) is a potentially useful alternative technique due to its speed, ease of use, and adaptability to on-line or off-line implementation. Not only has it been used to obtain structural information on cotton celluloses, but also it can be used to perform qualita-

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tive classification and quantitative prediction of cotton quality assessments. It has been successfully applied for the quantification of fiber moisture and chemical components (e.g., sugars) (Ghosh and Roy, 1988; Taylor and Godbey, 1994), for the prediction of color and physical attributes (e.g., reflectance, strength, micronaire, length, maturity, and uniformity) (Montalvo et al., 1994; Ramey, 1982; Rodgers et al., 2010; Thomasson and Shearer, 1995), for the detection of foreign contaminants (e.g., trash) (Taylor, 1980), for investigation of hydrogen bonding and crystallinity (Basch et al., 1974), and for characterization and discrimination of different cotton fibers (Liu et al, 1998a). Although these studies indicated that NIR spectroscopy is feasible and promising for quality evaluation of cotton fiber products, the results have been inconsistent. In addition, color is one of the most important fiber quality indices in cotton grading and classification, and few studies have been conducted by including the ultraviolet (UV) and visible regions.

Meanwhile, micronaire has been recognized as one of key cotton quality indices for fiber classifiers and processors (Heap, 2000). It is a measure of fiber fineness and maturity, and is determined by measuring the air permeability of a constant mass of cotton fiber compressed to a fixed volume. Previous studies have demonstrated the ability of NIR techniques to determine cotton micronaire with a relatively high degree of success (Montalvo et al., 1994; Thomasson and Shearer, 1995; Rodgers et al., 2010). Apparently, NIR-predicted micronaire values could be near the boundaries separating three cotton classes of “Discount Range,” “Base Range,” and “Premium Range” (USDA, 2001), which might be a problem and the source of error during cotton classification.

The main objective of this study was to examine the potential of NIR spectroscopy, with an extension to the UV/visible (220-750 nm) region, for the prediction of color and physical attributes of cotton fibers and for the comparison of micronaire classification efficiencies among three classes of cotton between two approaches: partial least-squares (PLS) regression, and soft independent modeling of class analogy of principal component analysis (SIMCA/PCA). The ultimate goal is to develop this technique for rapid, accurate, nondestructive, and routine determination of cotton fiber qualities in cotton fields, ginning sites, and classing offices.

Materials and Methods

Cotton Samples

A total of 123 cotton samples were used. Among them, 63 lint cotton samples were removed from different portions of 21 cotton bales that consisted of eight cotton varieties grown in three locations in the U.S. Cotton Belt and harvested in the 2001 crop year. An additional 60 samples were removed from different portions of six International Cotton Calibration standards (USDA Cotton Program, Memphis, Tenn.). This type of sampling of cotton fibers might be reasonable because cotton fibers from different locations of a bale (217.7 kg) have shown great variations in fiber properties (Van Dalfsen and Alberts, 1953; Bauer et al., 2009), and the obtained cotton micronaire readings cover most of the variability. Before testing, the samples from the 21 bales were cleaned on a Shirley analyzer (Shirley Developments, Ltd., Stockport, U.K.) in order to remove extraneous plant parts, and the samples from the calibration cottons were used as-is. Considering the fibers with and without the cleaning process, nearly equal numbers of samples from the two groups were utilized in the models. The cotton fibers were well conditioned at a constant relative humidity of 65% and temperature of 22°C ±2°C for at least 48 h prior to subsequent HVI and UV/visible/NIR spectral measurement.

Reference Measurement

Color and physical properties were measured by three modules of an Uster HVI 900A system (Zellweger Uster, Inc., Knoxville, Tenn.). The modules were calibrated routinely throughout the study using the manufacturer’s procedures. About 10 g of cotton fibers was, in turn, measured for micronaire by the micronaire module; Rd and +b were measured by the color/trash module; and strength, mean length, upper-half mean length, uniformity index, and short fiber index were measured by the length/strength module. Averages of multiple readings from each module were taken and used as references. Next, the identical pieces of samples were scanned for UV/visible/NIR reflectance.

UV/Visible/NIR Reflectance Measurement

Approximately 0.5 g of cotton fiber was pressed into an NIR sample cell, a cylinder shape of 1.0 cm depth and 5.0 cm diameter, and its larger surface was covered with an optically transparent glass window. The reflectance spectra were then scanned on a JASCO V-670 UV/visible/NIR spectrometer (JASCO, Eastern Shore, Md.) equipped with a diffuse-reflectance accessory that incorporates an ILN-725 150 mm integrating sphere. The system employs a photomultiplier tube detector for the 220-850 nm range and a PbS photoconductive detector for the 850-2500 nm range, with a respective bandpass of 5 and 20 nm. The background was recorded with a standard reference disk before collecting cotton reflectance spectra. The spectral measurements were acquired over the 220-2200 nm wavelength range at 1 nm interval. The reflectance (R) values were converted to log(1/R) values for data analysis.

Calibration and Validation Methods

All UV/visible/NIR spectra were imported into PLSplus/IQ package in Grams/AI (version 7.01, Thermo Fisher Scientific, Waltham, Mass.) and were smoothed with a Savitzky-Golay function (polynomial = 2 and points =13) prior to calibration and validation model development. All samples were ordered with the sequence of spectral acquisition (2001 crop year samples, and then international cotton calibration standards) and were random within each sample set. Of the 123 spectra, 82 were used for calibration equation development, and the remaining 41 (every third sample) spectra were used for model validation. To optimize the accuracy of the prediction models, the data were subjected to different combinations of both the spectral ranges, e.g., full and narrow regions, and the spectral pretreatments, e.g., mean centering (MC), multiplicative scatter correction (MSC), standard normal variate (SNV), and first and second derivatives. Full (one-sample-out rotation) cross-validation was used, and the number of optimal factors selected for the regression equation generally corresponded to the minimum of the predicted residual error sum of squares (PRESS). The saved regression equations were subsequently applied to the validation samples. Model accuracy and efficiency were assessed in the validation set on the basis of coefficient of determination (r^2), root mean square error of validation (RMSEV), and residual predictive deviation (RPD) (Williams, 2001). Generally, an optimal model should have lower RMSEV and higher r^2 and RPD.

Micronaire Classification Models

Classification models were also developed using the PLSPlus/IQ package. The assignment of calibration and validation samples in the classification model was the same as that in the prediction model. Briefly, 36 spectra representing the "Discount Range" cotton samples (measured micronaire less than 3.5 and greater than 5.0), 25 spectra representing the "Premium Range" cotton samples (measured micronaire between 3.6 and 4.2), and 21 spectra representing the "Base Range" cotton fibers (measured micronaire from 3.5 to 3.6 (no samples available at this work) and between 4.2 and 5.0) were used for discriminant model development. The additional 41 samples (18 "Discount Range," 10 "Premium Range," and 13 "Base Range") were used for the model validation. Classification models were established using three classes with mean centering (MC) spectral pretreatment in two spectral regions, 1100-2194 nm and 226-2194 nm, based on soft independent modeling of class analogy of principal component analysis (SIMCA/PCA) with spectral residuals. For each of the three classes in the two models, the optimal number of factors was suggested to be 7,7,7 and 8,8,8, respectively. By applying three SIMCA/PCA classes to the validation samples and employing the class assignment rule of the lowest spectral residuals, the sample was identified as belonging in the class being modeled, i.e., "Discount Range," "Base Range," or "Premium Range." One-out cross-validation was used as the validation method in SIMCA/PCA models.

Results and Discussion

UV/Visible/NIR Spectra of Cotton Fibers

Figure 1 shows the representative log(1/R) spectra of cotton fibers in the spectral region of 220-2200 nm. There are at least four intense and broad bands with one (<600 nm) in the UV/visible region (220-750 nm) and three (1490, 1935, and 2105 nm) in the NIR region (750-2200 nm). In this study, cotton fibers were either cleaned prior to analysis or were standard reference samples; thus, the interferences from foreign contaminants (such as botanical trash) could be minimal. In general, the UV/visible region of 220-750 nm contains the color information and represents a mixture of contributions from the pigmentation compounds present in cotton fibers, for example, flavonoids, and/or degraded products between a reducing sugar and an amino acid (Gamble, 2008; Hua et al., 2007), whereas the NIR bands are mainly due to the (1st and 2nd) overtones and combinations of OH and CH stretching vibrations of cellulose, which comprises more than 94% of cotton fiber mass. The broad bands between 1150 nm and 1300 nm are from the second overtones of CH stretching modes, and their first overtones appear in the 1675-1860 nm region (Burns and Ciurczak, 2001). Features in the 1300-1400 nm region are ascribed to combination bands of the CH vibrations. Broad and intense bands in the 1400-1675 nm region are due to the overlap of the first overtones of the OH stretching modes in hydrogen bonded forms. The strong bands at 1935 nm and 2105 nm are most likely attributable to the combination of OH stretching and deformation mode and the combination of OH and CO stretching vibrations in cellulose, respectively (Burns and Ciurczak, 2001).

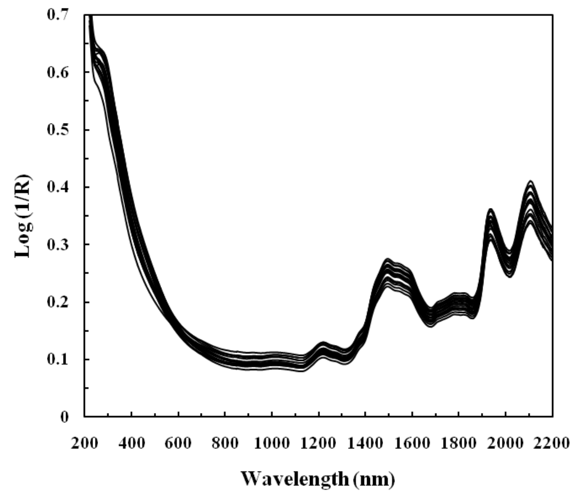

Figure 1. Representative UV/visible/NIR log(1/R) spectra of cotton fibers in the 220-2200 nm region.

Initial examination of all spectra revealed little intensity changes in the 220-2200 nm region with respect to specific cotton fiber qualities. In other words, UV/visible/NIR reflectance intensities in magnitude were not linear with specific fiber properties, although NIR models could predict some fiber qualities with high and promising accuracy (Ghosh and Roy, 1988; Montalvo et al., 1994; Ramey, 1982; Rodgers et al., 2010; Taylor and Godbey, 1994; Thomasson and Shearer, 1995). Actually, relatively large variations in UV/visible/NIR spectra were observed among the different sampling locations within the same variety (not shown). However, the spectra might still provide comprehensive information on chemical, physical, color, and structural properties in cotton fibers.

Pearson Correlation

Pearson correlations between pairs of eight separate quality indices are shown in table 1. In general, the eight fiber qualities could be considered as four types, color (Rd, degree of reflectance and +b, yellowness), fineness (as micronaire), strength, and length (as mean length and upper-half mean length, and the associated uniformity and short fiber indices were derived from the same HVI fibrogram). Besides the positive and moderate correlations with mean length, uniformity index, strength, and micronaire, Rd correlated with +b negatively and significantly and also with short fiber index negatively and moderately ($p < 0.05$). Meanwhile, +b, indicative of color pigmentation in cotton fibers, showed positive and moderate correlation with only one (short fiber index) of the other seven cotton attributes, indicating that both are related to low fiber quality. As expected, the four length properties had stronger correlations with each other than with color, micronaire, and strength. Meanwhile, it is relevant to point out the negative correlations between short fiber index and mean length, upper-half mean length, and uniformity index. Notably, little correlation was observed between strength and mi–

Table 1. Pearson correlations for eight fiber qualities from HVI measurement.[a]

	Rd	+b	ML	UHM	SFI	UI	STR	MIC
Rd								
+b	-0.59							
ML	0.24	-0.40						
UHM	0.18	-0.39	0.98					
SFI	-0.27	0.35	-0.86	-0.79				
UI	0.34	-0.24	0.63	0.47	-0.76			
STR	0.45	-0.39	0.51	0.48	-0.48	0.43		
MIC	0.20	-0.10	-0.15	-0.29	-0.15	0.47	0.01	

[a] ML = mean length, UHM = upper-half mean length, SFI = short fiber index, UI = uniformity index, STR = strength, and MIC = micronaire. Absolute values greater than 0.50 were subjectively considered to have significant correlation, values between 0.50 and 0.20 to have moderate correlation, and values less than 0.20 to have insignificant correlation.

Table 2. HVI reference values of range, mean, and standard deviation (SD) for eight fiber qualities in calibration and validation sets.

Cotton Characteristic	Calibration Set (n = 82)		Validation Set (n = 41)	
	Range	Mean ±SD	Range	Mean ±SD
Rd	72.97 - 84.80	78.08 ±2.68	72.97 - 84.80	78.23 ±2.65
+b	10.92 - 17.20	14.96 ±1.57	10.92 - 17.20	14.93 ±1.55
Mean length (inch)	0.692 - 0.964	0.853 ±0.069	0.700 - 0.964	0.857 ±0.066
Upper-half mean length (inch)	0.886 - 1.190	1.062 ±0.077	0.902 - 1.190	1.067 ±0.073
Short fiber index (%)	9.10 - 14.10	11.77 ±1.75	9.10 - 14.10	11.62 ±1.72
Uniformity index (%)	76.80 - 83.10	80.28 ±1.39	77.20 - 82.80	80.26 ±1.38
Strength (gm/tex)	22.84 - 36.15	28.55 ±3.08	24.11 - 36.39	29.12 ±3.16
Micronaire (units)	2.51 - 5.38	4.01 ±0.84	2.51 - 5.38	4.02 ±0.83

Table 3. Statistics in calibration and validation sets for eight cotton fiber qualities.[a]

Fiber Index	Spectral Region	Order of Spectral Pretreatment	Optimal Factors	Calibration Set (n = 82)		Validation Set (n = 41)		
				r^2	RMSEC	r^2	RMSEV	RPD
Rd	226-2194 nm	MC	8	0.90	0.86	0.82	1.13	2.3
	226-1100 nm	**MC + MSC + 1st der.**	**10**	**0.96**	**0.53**	**0.87**	**0.96**	**2.8**
	1100-2194 nm	MC	6	0.61	1.68	0.51	1.89	1.4
+b	**226-2194 nm**	**MC + MSC**	**7**	**0.96**	**0.30**	**0.96**	**0.31**	**5.0**
	226-1100 nm	MC	8	0.96	0.32	0.94	0.39	4.0
	1100-2194 nm	MC	5	0.82	0.66	0.82	0.66	2.3
Mean length	226-2194 nm	MC + MSC	7	0.82	0.029	0.78	0.031	2.1
	226-1100 nm	**MC + MSC + 1st der.**	**8**	**0.88**	**0.024**	**0.81**	**0.029**	**2.3**
	1100-2194 nm	MC	4	0.53	0.048	0.55	0.044	1.5
Upper-half mean length	226-2194 nm	MC + MSC	7	0.84	0.031	0.78	0.034	2.1
	226-1100 nm	**MC**	**9**	**0.84**	**0.031**	**0.82**	**0.031**	**2.3**
	1100-2194 nm	MC + MSC	4	0.62	0.048	0.59	0.047	1.5
Short fiber index	**226-2194 nm**	**MC + MSC + 1st der.**	**4**	**0.82**	**0.75**	**0.75**	**0.87**	**2.0**
	226-1100 nm	MC + MSC	7	0.71	0.95	0.71	0.94	1.9
	1100-2194 nm	MC + 1st der.	2	0.52	1.21	0.55	1.15	1.5
Uniformity index	**226-2194 nm**	**MC**	**9**	**0.78**	**0.66**	**0.76**	**0.69**	**2.0**
	226-1100 nm	MC	8	0.66	0.82	0.74	0.71	1.9
	1100-2194 nm	MC	2	0.38	1.11	0.49	1.01	1.4
Strength	226 -2194 nm	MC + 1st der.	4	0.74	1.59	0.55	2.25	1.4
	226-1100 nm	**MC**	**12**	**0.74**	**1.59**	**0.63**	**2.11**	**1.5**
	1100-2194 nm	MC	4	0.31	2.58	0.20	2.91	1.1
Micronaire	226-2194 nm	MC	7	0.97	0.14	0.97	0.14	5.9
	226-1100 nm	MC	12	0.96	0.17	0.91	0.25	3.3
	1100-2194 nm	**MC**	**4**	**0.97**	**0.15**	**0.98**	**0.13**	**6.4**

[a] MC = mean centering, MSC = multiplicative scatter correction, 1st der. = first derivative, RMSEC = root mean square error of calibration, RMSEV = root mean square error of validation, and RPD = residual predictive deviation. The best model for each fiber quality is shown in **boldface** type.

cronaire. Existence of correlations between two color parameters and other fiber physical properties suggested that the development of cotton color is probably associated with at least one of the fiber physical properties during the cotton growth and maturity.

Reference Values

Table 2 summarizes the range, mean, and standard deviation (SD) of reference values for color and physical attributes of cotton fibers in the calibration and validation sets. The variations of reference values covered most of the variability in fiber properties (Montalvo et al., 1994; Rodgers et al., 2010; Thomasson and Shearer, 1995). The range, mean, and SD values for an individual property were similar within the calibration and validation sets, indicating that the selection of samples for each set was appropriate.

Calibration and Prediction Models

Partial least-squares (PLS) regression models for all properties were developed using the different combinations of full/narrow spectral regions and a variety of data pretreatments. The statistics of optimal results in the calibration and validation sets from three spectral regions are summarized in table 3. In addition to the entire 226-2194 nm region, the log(1/R) spectra were analyzed subjectively in two narrow regions: 226-1100 and 1100-2194 nm. The reasons for choosing these spectral regions were (1) to compare the model performances from different spectral regions, and (2) to facilitate the development of portable optical and spectral imaging sensors in either the visible or NIR region (Jia and Ding, 2005; Sui et al., 2008). For each property in a specific spectral region, the optimal model was determined by lower RMSEV and higher r^2 in the validation set, respectively.

Table 3 shows that the best prediction models were obtained from the combinations of such spectral pretreatments as MC, MSC, and first derivative on previously smoothed spectra. The use of second derivative, along with other data processing, yielded much poorer results for all properties (not shown). This observation is in good agreement with that reported by Montalvo et al. (1994). Comparison of the RMSEV and r^2 values in the validation set indicated that the models from the full region (226-2194 nm) produced the optimal predictions for +b, short fiber index, and uniformity index. The models representing the 226-1100 nm region yielded the best results for Rd, mean length, upper-half mean length, and strength, and the model in the 1100-2194 nm NIR region had the best performance for micronaire. Notably, the optimal models for fiber properties agreed very well with the Pearson correlations from the HVI values in table 1. For instance, micronaire, with the best model from the 1100-2194 nm NIR region, had much lower correlation with two color indices than strength and lengths, which had the best models from the region including the UV/visible absorptions.

Examination of the RMSEC, RMSEV, and r^2 values in table 3 also suggests that micronaire could be predicted closely by two models, either from the full region (226-2194 nm) or from the 1100-2194 nm NIR region. Together with other models, this indicated that all cotton properties could be best assessed by the utilization of the entire UV/visible region. Meanwhile, the predictive models in table 3 were similar to or better than those previously reported (Montalvo et al., 1994; Thomasson and Shearer, 1995), in which the "dissimilar" samples were removed from calibration and validation sets by cluster analysis or the optimum regression models were not validated by independent samples.

RPD, the ratio of the standard deviation (SD) of a reference value to the root mean square error of validation (RMSEV), is often used as a dimensionless gauge of the ability of a spectroscopic model to predict a property (Williams, 2001). An RPD value of greater than 2.5 indicates that the spectroscopic model might be suitable for screening programs, and a value of greater than 5.0 is potentially useful in quality control. From the scale of RPD values in table 3, the models for micronaire and +b as well as for Rd could be used for quality control and screening applications, respectively.

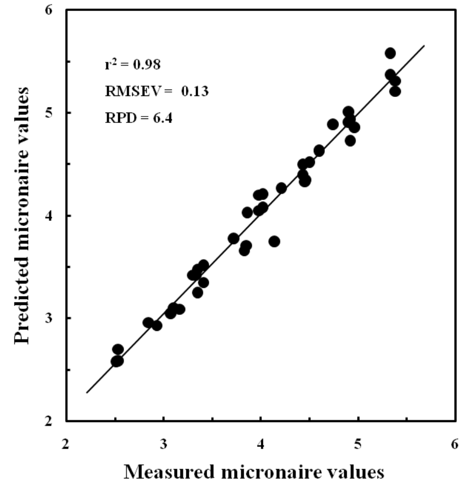

Figure 2. Correlation plot of measured vs. UV/visible/NIR-predicted micronaire.

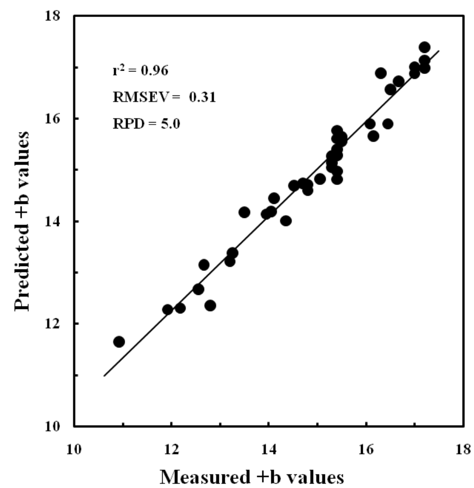

Figure 3. Correlation plot of measured vs. UV/visible/NIR-predicted +b.

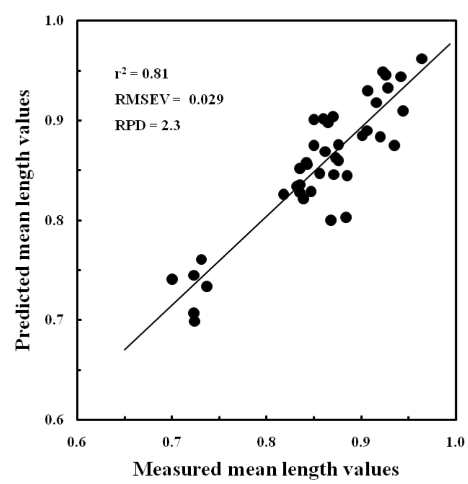

Figure 4. Correlation plot of measured vs. UV/visible/NIR-predicted mean length.

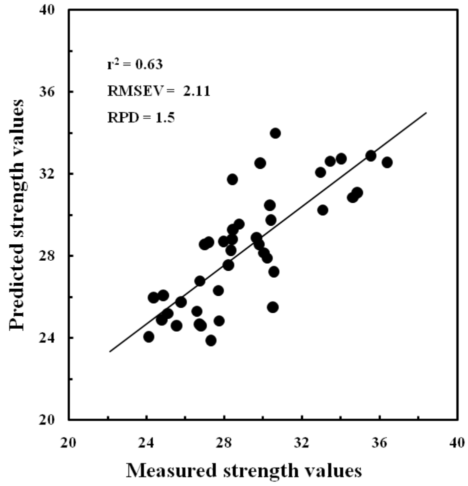

Figure 5. Correlation plot of measured vs. UV/visible/NIR-predicted strength.

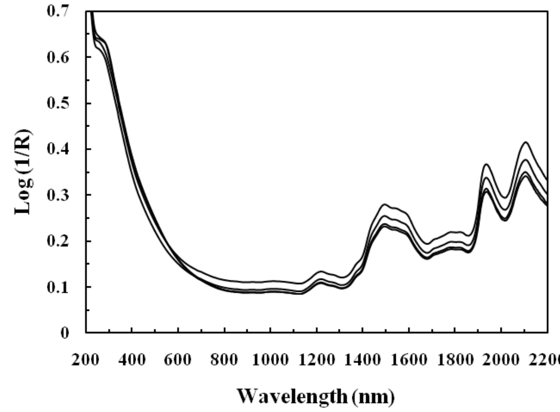

Figure 6. Representative UV/visible/NIR log(1/R) spectra of cotton fibers in the 220-2200 nm region at micronaire readings of <3.5, 3.5-4.2, 4.3-5.0, and >5.0, from bottom to top.

With RPD values not greater than 2.0, the strength, short fiber index, and uniformity index could not be modeled as effectively as other fiber indices investigated.

Among the eight attributes, the feasibilities of UV/visible/NIR predictive models could be in the descending order of micronaire, +b, Rd, mean length and upper-half mean length, uniformity index, short fiber index, and strength. Examples of plots for the measured vs. UV/visible/NIR predicted values in the validation set are shown in figures 2 through 5 for micronaire, +b, mean length, and strength, respectively. These plots suggest how well the UV/visible/NIR models work for the reference values from HVI measurements.

Spectral Response and Fiber Quality Characteristics

Within the 41 validation samples in the micronaire, mean length, and strength models, there were 1, 6, and 8 samples that had prediction error (or difference) greater than the permitted ranges of 0.30 units, 0.04 inches, and 3.00 gm/tex (USDA, 2005), respectively. Among these samples, none was observed simultaneously in the models for micronaire, mean length, and strength, and only one was common in the models for mean length and strength. This indicated that the prediction difference probably was not from the UV/visible/NIR spectral measurement in this study. Instead, most likely it resulted from the degree of precision and reliability in determining the reference value and the lack of specific property information in this region. There is a possibility that the outlier predictions could actually be real, that is, they were caused by the chemical or physical nature of the sample itself.

The above results suggest that micronaire and +b could be more easily and accurately predicted than other fiber indices, with the most difficult prediction being for strength. Micronaire is a function of wall thickness and perimeter, and is related with the relative proportion of the fiber's cellulose component to total fiber mass, while +b is indicative of fiber yellowness originating from organic chromophores and exhibits the characteristic chlorophyll and carotenoid bands in specific NIR or UV/visible regions. On the other hand, fiber strength and fiber lengths might be better determined by the factors that cannot be obtained by UV/visible/NIR spectral absorptions. In an earlier study, PC2 scores from principal component analysis (PCA) of FT-Raman spectra of various cotton fibers were found to have a link with the strength of the cotton fibers (Liu et al., 1998b). Therefore, improvement in HVI reference measurement and use of other vibrational spectroscopic tools, such as IR and Raman, should be examined in the future.

Micronaire Classification Model

Figure 6 shows the representative micronaire-dependent log(1/R) spectra of cotton fibers in the spectral region between 220 and 2200 nm by averaging the spectra of neighboring micronaire values in the respective range of <3.5, 3.5-4.2, 4.3-5.0, and >5.0. Although it suggests that cotton fibers with low micronaire have NIR bands in common with fibers having high micronaire, there appear to be some intensity variations induced by the micronaire index, for example, changes in relative intensity and position of UV/visible bands (<750 nm) and baseline shifting at the high-wavelength wing (>750 nm). Such fluctuations reflect the chemical, physical, structural, and color variations among cottons and could be associated with the fiber's fineness and maturity (Montalvo and Von Hoven, 2005).

Cotton fibers were assigned into "Discount Range," "Base Range," and "Premium Range" classes according to predicted micronaire values from previous optimal PLS models. Table 4 summarizes the classification results for the validation data set using the established criterion (USDA, 2001). Of the 18, 13, and 10 cotton samples considered as "Discount Range," "Base Range," and "Premium Range," 16, 12, and 9 samples were correctly classified in their respective classes by the PLS model from the 1100-2196 nm NIR region, with a 90.4% of overall classification. The use of optimal PLS models from the 226-2196 nm full region slightly improved the accuracy of correct identification from 90.4% to 91.1%. Further examination of the misclassifications revealed that all of them arose from the boundary samples, which obviously is reasonable and would be a problem in determining the fiber class assignment. Hence, besides the effort of improving the PLS prediction model, an innovative spectral processing strategy might be necessary.

For comparison, the 3-class based SIMCA/PCA discriminant models for the same data set were developed, and the results are also given in table 4. Unlike the PLS model, SIMCA/PCA only utilizes the spectral information and does

Table 4. Three-class classification of "Discount Range," "Base Range," and "Premium Range" cotton fibers in validation set (*n* = 41) from UV/visible/NIR reflectance based on predicted and measured micronaire values.

Model[a]	Correct Classification (%) "Discount Range"	"Base Range"	"Premium Range"	Average[b] (%)
PLS				
1100-2194 nm	88.9	92.3	90.0	90.4
226-2194 nm	83.3	100	90.0	91.1
SIMCA/PCA				
1100-2194 nm	88.9	84.6	70.0	81.2
226-2194 nm	100	100	100	100

[a] Spectral pretreatment with mean centering (MC) only.
[b] Mean of % correct classification for "Discount Range," "Base Range," and "Premium Range" classes.

not involve the actual micronaire readings during the model development. It is encouraging to observe a more enhanced classification from the SIMCA/PCA model in the 226-2194 nm region than in the 1100-2194 nm NIR region. The result also indicates that the classification from SIMCA/PCA model is better than that from PLS model in the same 226-2194 nm region, reaching a perfect separation.

Conclusions

The results of the present study demonstrate the usefulness of UV/visible/NIR spectroscopy in the characterization and determination of cotton fiber qualities. Pearson correlations among two color and six physical attributes from HVI measurement indicated several significant or moderate correlations. PLS regression models from the spectra and HVI data were individually developed in three spectral regions. The best models for nearly all properties were obtained with the inclusion of the UV/visible region and corresponded well with the Pearson correlations from the HVI data alone, indicating the importance of cotton color in the characterization of other cotton physical properties. Meanwhile, the results suggested that UV/visible/NIR models can be used to predict micronaire and +b for quality control applications, and to assess Rd for screening programs. However, for strength, more work is needed to reflect the spectral response and/or improve the reference method. On the basis of a small number of samples, this study indicated a proof of concept, and a larger study is under the way.

To reduce the likelihood of misclassifying the boundary samples from the PLS-predicted micronaire values, 3-class SIMCA/PCA models are developed, and the correct classifications were compared between two approaches. Results indicated that the discrimination model from the 226-2194 nm region could distinguish one type of cotton fiber from the other two classes at a satisfactory and perfect level. This finding is most promising in the development of spectral sensing system for *in situ* measurement of cotton micronaire at cotton fields and processing sites.

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